

# Phase transition in a 2-dimensional Heisenberg model

Henk W. J. Blöte <sup>†,‡</sup>, Wenan Guo <sup>§</sup> and Henk J. Hilhorst <sup>\*</sup>

<sup>†</sup> *Faculty of Applied Sciences, Delft University of Technology,  
P.O. Box 5046, 2600 GA Delft, The Netherlands*

<sup>‡</sup> *Lorentz Institute, Leiden University, P.O. Box 9506, 2300 RA Leiden, The Netherlands*

<sup>§</sup> *Physics Department, Beijing Normal University, Beijing 100875, P. R. China*

<sup>\*</sup> *Laboratoire de Physique Théorique, Bâtiment 210, Université de Paris-Sud,  
91405 Orsay, France  
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We investigate the two-dimensional classical Heisenberg model with a nonlinear nearest-neighbor interaction  $V(\vec{s}, \vec{s}') = 2K[(1 + \vec{s} \cdot \vec{s}')/2]^p$ . The analogous nonlinear interaction for the XY model was introduced by Domany, Schick, and Swendsen, who find that for large  $p$  the Kosterlitz-Thouless transition is preempted by a first-order transition. Here we show that, whereas the standard ( $p = 1$ ) Heisenberg model has no phase transition, for large enough  $p$  a first-order transition appears. Both phases have only short range order, but with a correlation length that jumps at the transition.

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The two-dimensional Heisenberg and XY model are such close relatives that it has taken a long history of efforts before their properties could be told apart. Both are special cases, for  $n = 3$  and 2, respectively, of the  $O(n)$  symmetric Hamiltonian

$$\mathcal{H} = -K \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j \quad (1)$$

Here  $\vec{s}_i$  is an  $n$ -component spin of unit length at lattice site  $i$ , the sum is on all pairs of nearest-neighbor sites of a two-dimensional lattice, and  $K = J/k_B T$ . For all  $n > 1$  the system (1) has  $d = 2$  as its lower critical dimension.

Bloch's 1930 spin wave argument [1], put on a firm mathematical basis only much later by Mermin and Wagner [2,3], implies that neither the XY nor the Heisenberg model can have a spontaneously magnetized low- $T$  phase. The early investigations dealt exclusively with the Heisenberg model. In 1958 Rushbrooke and Wood, after studying high- $T$  series [4], first remarked that in spite of Bloch's argument the possibility of a phase transition in the Heisenberg model should be taken seriously. This was reemphasized in 1966 by Stanley and Kaplan [5], who envisage, for the *Heisenberg* model, a low- $T$  phase with an infinite susceptibility.

In the late 1960's the high- $T$  series of the Heisenberg the XY model were compared [6,7]. Qualitative similarity was found, but no general agreement was ever reached about the significance of certain quantitative differences. A phase transition in either model continued to be considered by many as only a remote possibility, until Kosterlitz and Thouless (KT) [8] demonstrated that there *is* a phase transition in the *XY model* and clarified its topological character.

Since the KT arguments were specific for  $n = 2$ , the two-dimensional Heisenberg model (and, indeed, the Hamiltonian (1) for all  $n > 2$ ) has from then on been believed to be without a transition. Further support for this view came from the analytical low- $T$  renormalization group approach developed by Polyakov [9], Brézin and Zinn-Justin [10], and Nelson and Pelcovitz [11], and from Monte Carlo renormalization due to Shenker and Tobochnik [12]. The absence of a rigorous proof has however left room for arguments ([13] and references therein) that the Heisenberg model (Eq. (1) with  $n = 3$ ) may after all have a phase transition; this is not, however, our point of view.

Here we consider the  $O(3)$  symmetric Hamiltonian

$$\mathcal{H} = - \sum_{\langle i,j \rangle} V(\vec{s}_i \cdot \vec{s}_j) \quad (2)$$

where  $V$  is an arbitrary nonlinear function. For reasonable choices of  $V$  (in a sense not *a priori* clear) one expects that (2) is in the same universality class as the standard "linear"  $O(n)$  model (1). Expression (2) is interesting for at least two reasons.

First, the freedom to choose  $V$  is a key ingredient in theoretical analyses by Villain [14] of the  $O(2)$  model and by Domany *et al.* [15] and Nienhuis [16] of the  $O(n)$  loop model. For  $n > 2$  the latter model does undergo a phase transition [17] which corresponds to a hard-hexagon-like ordering of the loops. But in spin language the transition

appears to occur in an unphysical parameter region with negative Boltzmann weights. It does not provide evidence for a phase transition in  $O(n)$  spin models with  $n > 2$ .

The second reason of interest in (2) comes from the relevance of the KT theory for the melting of thin adsorbed layers. The difficulty encountered in observing the predicted [18] hexatic phase, whether experimentally or in simulations, was suspected by some to be due to the KT transition being preempted by a first order transition as a consequence of various nonlinearities not incorporated in the theory. Domany et al. (DSS) [19] therefore investigated an  $O(2)$  symmetric XY model with a specific nonlinearity controlled by a parameter  $p$ , *viz.*

$$V(\vec{s}_i \cdot \vec{s}_j) = 2K[(1 + \vec{s}_i \cdot \vec{s}_j)/2]^p \quad (3)$$

(our  $p$  is their  $p^2$ ). Indeed DSS found by Monte Carlo simulations that for strong enough nonlinearity ( $p \sim 50$ ) the KT transition is replaced with a first-order one from the massless low- $T$  phase to a high- $T$  phase with exponentially decaying correlations. While this suggests that melting via a hexatic phase may similarly be preempted by a first-order transition, the DSS result has been subject to controversy [20].

Here we confront again the XY and Heisenberg model. We have Monte Carlo simulated the latter with the nonlinear interaction (3) on square  $L \times L$  periodic lattices. Randomly chosen orientations are accepted with Metropolis-type probabilities. Slow relaxation at low  $T$  limits the largest system size to about  $L = 200$ .

No signs of a phase transition were seen for  $p \approx 1$ , but for  $p = 20$  there is a clear jump in the energy as a function of  $K$ . Fig. 1 shows the resulting hysteresis for a system of size  $L = 48$ . For the XY model a similar narrow hysteresis loop was observed by DSS, but today's computers yield a clearer picture in the Heisenberg case.

Similar Monte Carlo runs for  $p < 20$  show a weaker first-order character, but do not clearly show where the first-order line ends. In order to answer this question, we have determined the specific heat for a grid of points in the  $K$ - $p$  plane. We thus found the specific-heat maxima as a function of  $K$ . Fig. 2 displays these maxima  $C_{\max}(p, L)$  versus  $L$ . In the absence of a phase transition  $C_{\max}(p, L) \simeq \text{cst}$  when  $L$  increases; this behavior is seen for small  $p$ . In its presence we expect, at large  $L$ ,

$$C_{\max}(p, L) \simeq c_0 L^{2y-2} \quad (4)$$

with  $y = 2$  ( $y < 2$ ) in the case of a first-order (continuous) transition. The data for  $p = 20$  in Fig. 2 are consistent with  $y = 2$ . The finite-size divergence weakens for  $p < 20$ , and the  $p = 16$  data indicate a continuous transition with  $y = 1.84 \pm 0.05$ . The downward trend at even smaller  $p$  is consistent with  $C_{\max}(p, L) \simeq \text{cst}$  at large  $L$ . This suggests that the first-order line in the  $p$ - $K$  diagram ends in a critical point near  $p = 16$ .

Simulations for  $p > 20$  show an enhanced first-order character. Transition points were found by several runs, starting with half the system fully aligned, and the other half chosen randomly. The results, which hardly depend on  $L$  for  $L > 32$ , are shown in Fig. 3 versus  $p$ .

The transition points can also be estimated from the high- and low- $T$  expansions of the free energy. Neglecting loop diagrams in the high- $T$  expansion the lattice effectively reduces to the Bethe lattice (BL). Its partition function 'per bond' is

$$\int d\vec{s} \exp 2K[(1 + \vec{s} \cdot \vec{t})/2]^p = 4\pi \sum_{k=0}^{\infty} \frac{(2K)^k}{(1 + pk)k!} \quad (5)$$

where the prefactor accounts for the phase space volume of a spin and the sum for the spin-spin interaction. For  $N$  spins and  $zN/2$  bonds we thus have

$$Z_{\text{BL}} = (4\pi)^N \left( \sum_{k=0}^{\infty} \frac{(2K)^k}{(1 + pk)k!} \right)^{zN/2} \quad (6)$$

which yields the high- $T$  approximation  $F_{\text{HT}}$  of the free energy of a square lattice ( $z = 4$ ) of  $N = L^2$  sites as

$$\frac{F_{\text{HT}}}{Nk_B T} = -\log(4\pi) - 2 \log \left( \sum_{k=0}^{\infty} \frac{(2K)^k}{(1 + pk)k!} \right) \quad (7)$$

At low  $T$ , the spin-wave approximation (SWA) of  $\mathcal{H}$  is

$$\mathcal{H}_{\text{SWA}}(\{\vec{s}_i\}) = -4NK + \mathcal{H}_G(\{s_i^x\}) + \mathcal{H}_G(\{s_i^y\}) \quad (8)$$

where  $\mathcal{H}_G$  is the Gaussian Hamiltonian

$$\mathcal{H}_G(\{s_i\}) = \frac{1}{2}pK \sum_{\langle ij \rangle} (s_i - s_j)^2 \quad (9)$$

By standard methods one obtains from it the low- $T$  approximation  $F_{LT}$  to the free energy,

$$\begin{aligned} \frac{F_{LT}}{Nk_B T} &\simeq -4K - \log(4\pi) + \log(8pK) \\ &+ \frac{1}{N} \sum'_{m,n=0}^{L-1} \log[(\sin \frac{\pi m}{L})^2 + (\sin \frac{\pi n}{L})^2] \end{aligned} \quad (10)$$

where the prime indicates that  $(m, n) = (0, 0)$  is excluded from the sum. For large  $N = L^2$  the sum on  $m$  and  $n$  tends towards  $-2\log 2 + 4G/\pi = -0.2200507 \dots$  where  $G$  is Catalan's constant.

The intersection of the two free-energy branches was found numerically for several  $p$ . The resulting approximation of the first-order line, shown in Fig. 3, is in a good qualitative agreement with the Monte Carlo results.

Next, we check the consistency of our magnetization data for the low- $T$  phase with the Mermin-Wagner theorem [2,3]. Fig. 4 shows that the mean square magnetization  $m^2 \equiv L^{-4} \sum_i \sum_j \langle \vec{s}_i \cdot \vec{s}_j \rangle$  decays slowly with  $L$ . In contrast, the energy rapidly tends to a constant with increasing  $L$ .

In order to compare this magnetization behavior to theory, we recall that in the standard ( $p = 1$ ) Heisenberg model the correlation length  $\xi$  is well fitted [12] at low  $T$  by  $\xi(K) \approx C \exp(2\pi K)/(1+2\pi K)$  with  $C \approx 0.01$ . For  $1 \ll r \lesssim \xi$  one expects the SWA result  $g(r) \equiv \langle \vec{s}_i \cdot \vec{s}_{i+r} \rangle \sim r^{-\eta}$  to hold, where  $\eta = 1/\pi K$ . Consequently  $m^2 \sim L^{-2} \int_0^L dr r g(r) \sim L^{-\eta}$  for  $1 \ll L \lesssim \xi$ . For  $\xi \lesssim L$  the integral on  $r$  converges at the upper limit and one has  $m^2 \sim L^{-2}$ .

Now take  $p \gg 1$  in the model under study. Then the angle  $\theta$  between two neighboring spins is in a narrow two-dimensional harmonic potential well as long as  $\theta \ll \pi p^{-1/2}$ . For  $\pi p^{-1/2} \lesssim \theta$  the Boltzmann weight is decreased by a factor  $\exp(-2K)$  and almost independent of  $\theta$ . When  $K \gg 1$ , most angles are small, and  $g(r)$  will behave according to the SWA, but with an exponent  $\eta = 1/\pi p K$ ; and the correlation length  $\xi(pK)$  estimated as above will exceed any system size  $L$  attainable in simulations (disregarding a renormalization effect of  $\xi$  due to the nonlinearity of  $V$ ).

Next let  $K \sim 1$  while still  $pK \gg 1$ . Then the fraction of nearest neighbor spins with large relative angles will no longer be exponentially small in  $K$ . This will cause a downward renormalization of the effective coupling of the SWA, if this concepts remains at all applicable, and of  $\xi$ , but it is not *a priori* clear if  $\xi$  will still exceed the system size. To answer this question we consider Fig. 4. For  $p = 20$  and  $K = 1.4$  the unrenormalized SWA gives  $\eta = 1/\pi p K = 0.012$ . Fig. 4 confirms the power law decay of  $m^2$ , but yields a renormalized exponent  $\eta_{\text{eff}} \approx 0.030$ , estimated from the range  $32 \leq L \leq 192$ . This corresponds to an effective SWA coupling  $K_{\text{eff}} \approx 10.6$ . We note that  $\xi(K_{\text{eff}})$  is still very much larger than our  $L$  values, which indicates the self-consistency of the renormalized SWA. Hence we conclude that the low- $T$  phase has a correlation length  $\xi$  much larger than the system sizes  $L$  considered here, and has a pair correlation that, at these distances, decays as a power law.

Our finite sizes  $L$  restrict the spin waves to small deviations, so that  $m^2$  is considerable. One may ask how stable the first-order transition is under large deviations occurring in large systems. We have imposed large-amplitude waves using antiperiodic boundaries in both directions. This reduces  $m^2$  considerably in finite systems at low- $T$ , and renders the low- $T$  phase less stable. Monte Carlo data at  $p = 20$ ,  $L = 48$  show that the energy jump and hysteresis are strongly suppressed. The deformation energy per bond is  $\propto L^{-2}$ . Fig. 5 shows that for  $L = 192$  indeed the first-order character is partly restored to the situation of Fig. 1. This indicates that the first-order transition persists even when spin waves suppress the magnetization at large  $L$ .

It is not clear how to define an order parameter reflecting a symmetry of the model. The phases separated by the first-order line have different degrees of short-range order, as is the case in a gas-liquid system. Thus we expect the first order line to end in an Ising-like critical point. Indeed, our result  $y = 1.84 \pm 0.05$  agrees well with the Ising magnetic exponent  $y_h = 15/8$ . We note that the energy fluctuations of this model correspond with the Ising *magnetic* scaling field, because it is the energy that has a discontinuity at the first-order line.

In conclusion, we have investigated a Heisenberg model with interactions that depend nonlinearly on the spin products. For strong enough nonlinearity there appears a phase transition. This transition is unrelated to earlier claims [13], which applied to the linear case. But it does seem related to the DSS transition in the XY model in the following way. Adding a term  $\gamma \sum_k (s_k^z)^2$  in Eq. (2) leads to crossover to the O(2) model as  $\gamma$  varies from 0 to  $\infty$ . In the  $\gamma p$  plane we expect a line  $p = p_c(\gamma)$  (with  $p_c(0) \approx 16$ ) above which the transition is first order and below which it is of the KT type when  $\gamma > 0$ .

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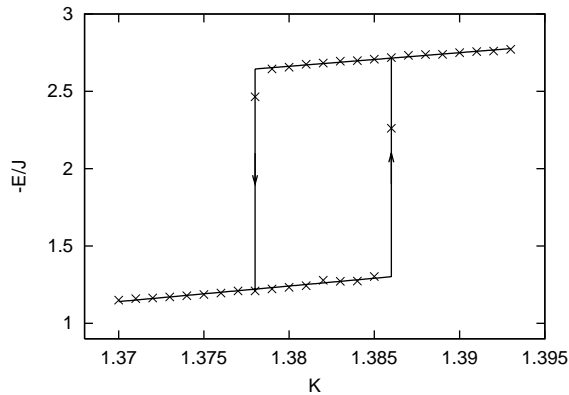


FIG. 1. Energy per spin versus coupling for a periodic system of size  $L = 48$  and  $p = 20$ . The energy discontinuity and the hysteresis indicate a first-order phase transition. Each data point results from  $10^6$  Monte Carlo steps per site. The statistical errors are smaller than the symbol size. Jumps in the energy (see arrows) occurred while taking the data points on the vertical lines.

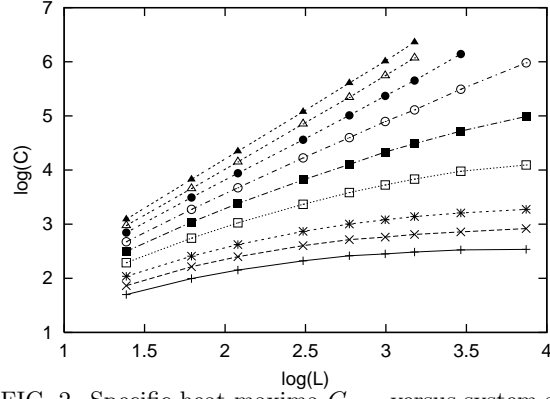


FIG. 2. Specific-heat maxima  $C_{\max}$  versus system size  $L$  on logarithmic scales. The curves serve only to guide the eye. The data points apply to  $p = 6$  (+),  $p = 7$  (x),  $p = 8$  (\*),  $p = 10$  (□),  $p = 12$  (■),  $p = 14$  (○),  $p = 16$  (●),  $p = 18$  (△), and  $p = 20$  (▲). These data suggest that the critical point at the end of the first-order line lies near  $p = 16$ . Each data point was determined from several Monte Carlo runs which, because of slow relaxation, had to be long (up to about  $10^8$  updates per site each). This is where the bulk of the computational effort went. The errors do not exceed the symbol size.

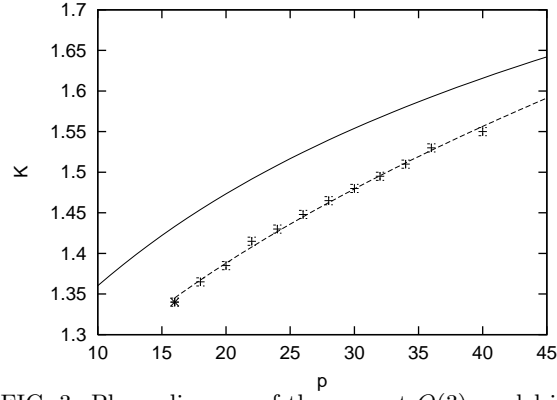


FIG. 3. Phase diagram of the present  $O(3)$  model in the  $p$  vs.  $K$  plane. The full curve is obtained by equating the high- $T$  and the low- $T$  expansions of the free energy. The data points represent our numerical results.

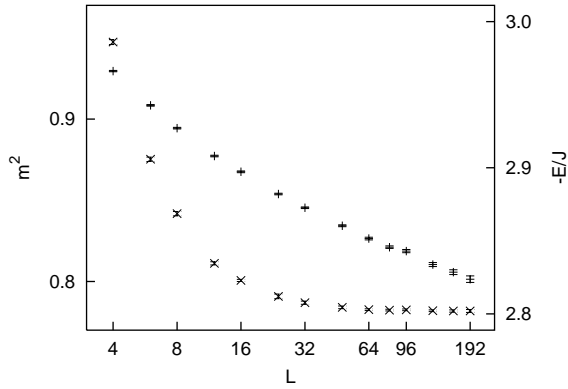


FIG. 4. Magnetization squared (+) and energy(x) per spin versus system size  $L$  in the low- $T$  phase at  $K = 1.4$ ,  $p = 20$ .

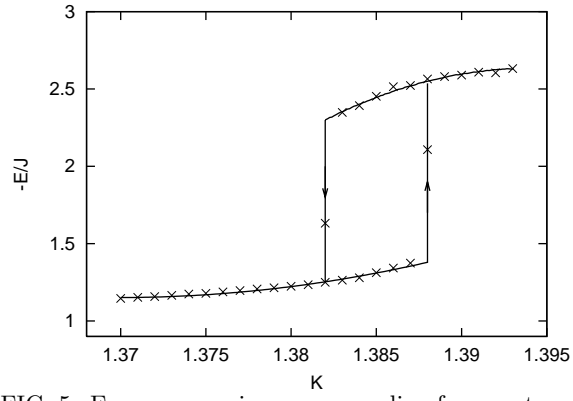


FIG. 5. Energy per spin versus coupling for a system of size  $L = 192$  and  $p = 20$  with antiperiodic boundary conditions. The first-order character is still apparent under these conditions. Each data point represents a simulation of  $2 \times 10^5$  Monte Carlo steps per site. The statistical errors are comparable to the symbol size.